

A_+/A_- , α , ν , and $f_s \xi^3$ from 3D Ising Energy and Specific Heat

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Abstract

We analyse Monte Carlo data for the energy and specific heat at and close to the critical point of the 3D cubic Ising model. From the finite size scaling of the energy E and the specific heat C at criticality we obtain the estimate $\nu = 0.6308(10)$. Furthermore, one obtains precise estimates for the “backgrounds” (nonsingular parts) E_{ns} and C_{ns} . Fitting solely off critical energy estimates to a scaling law, we find, depending on the choice of the reduced temperature, either $A_+/A_- = 0.550(12)$ and $\alpha = 0.1115(37)$, or $A_+/A_- = 0.567(16)$ and $\alpha = 0.1047(48)$. Including information from the data at T_c , we obtain the estimate $A_+/A_- = 0.560(10)$. We also determine the universal combination $f_s \xi^3$ in both phases.

The universal amplitude ratio A_+/A_- of the 3D Ising universality class (for a precise definition see eq. (6) below) still seems subject to some uncertainty. For a general discussion of the difficulties one encounters when trying to estimate A_+/A_- from high and low temperature expansions see ref. [1]. A compilation of some results in the literature will be given in the last section of this article. For a general introduction to universal critical-point amplitudes see e.g. [2].

We here present a calculation of A_+/A_- based on Monte Carlo data for the energy of the 3D Ising model. Furthermore, we obtain fairly precise estimates of other quantities, like the exponents ν and α , nonsingular parts of energy and specific heat, and of the universal combination $f_s \xi^3$ on both sides of the transition.

Consider the 3D Ising model on the simple cubic lattice of size $L \times L \times L$, with periodic boundary conditions. The Hamiltonian is

$$H = - \sum_{\langle x,y \rangle} s_x s_y, \quad s_x = \pm 1. \quad (1)$$

The sum in eq. (1) is over all (unordered) nearest neighbour pairs of sites in the lattice. The partition function is

$$Z = \sum_{\{s\}} \exp(-\beta H). \quad (2)$$

Here, the summation is over all possible configurations of the Ising spins. The pair interaction is normalised such that $\beta = 1/(k_B T)$, where k_B denotes Boltzmann's constant, and T is the temperature.

At a critical coupling $\beta_c = 0.2216544(6)$ [3] the model undergoes a second order phase transition. For $\beta > \beta_c$, the system shows spontaneous breaking of reflection symmetry.

The free energy density (free energy per link) is defined by

$$f = -\frac{1}{3L^3} \ln Z. \quad (3)$$

We define the energy (per link) as the derivative of f with respect to β ,

$$E = -\frac{d}{d\beta} f = -\frac{1}{3L^3} \langle H \rangle. \quad (4)$$

The specific heat is defined as the derivative of E with respect to β ,

$$C = \frac{d}{d\beta} E = \frac{1}{3L^3} \left(\langle H^2 \rangle - \langle H \rangle^2 \right). \quad (5)$$

Note that choosing other definitions, like putting a minus sign in eq. (4) or substituting a d/dT instead of the $d/d\beta$ in eq. (5) leads to trivial factors and/or signs in the definitions and results to be stated below.

The specific heat is singular at the critical point. Close to β_c it is expected to behave like

$$C \simeq C_{\text{ns}} + C_s, \quad (6)$$

where C_{ns} is an analytic function of β at β_c . The singular part is

$$C_s \simeq A_{\pm} |t|^{-\alpha}, \quad (7)$$

where

$$t = 1 - \frac{\beta}{\beta_c} \quad (8)$$

is the reduced temperature. A_+ and A_- denote the amplitudes of the singular part in the symmetric ($t > 0$) and broken ($t < 0$) phase, respectively. α is the specific heat exponent. The singularity of the specific heat implies a non-analytic behaviour of the energy E and the free energy density f . Some details will be given in the next section.

1 Scaling and Finite Size Scaling

For a general introduction to finite size scaling theory, see, e.g., ref. [4]. In order to discuss the non-analytic behaviour of the free energy density it is useful to split it into an analytic (nonsingular) and a singular part,

$$f = f_{\text{ns}} + f_s. \quad (9)$$

Renormalization group arguments lead to the following finite size scaling ansatz for the singular part of the free energy density for lattices with periodic boundary conditions [5],

$$f_s \xi^d \simeq g(\xi/L), \quad (10)$$

where f_s is taken in the finite volume, while ξ is the correlation length defined in the thermodynamic limit. $g(\xi/L)$ is a universal function. In the following we discuss the two extremal cases of the thermodynamic limit and the finite size scaling exactly at the critical point.

The thermodynamic limit is characterised by $\xi/L = 0$. Inserting the scaling ansatz $\xi \sim t^{-\nu}$ into eq. (10) for $\xi/L = 0$ we obtain

$$f_s \sim t^{d\nu}. \quad (11)$$

By differentiation with respect to β we arrive at

$$E_s \sim t^{d\nu-1} \quad (12)$$

and

$$C_s \sim t^{d\nu-2}. \quad (13)$$

The last equation implies the so called hyperscaling relation $\alpha = 2 - d\nu$.

In order to discuss finite size scaling at the critical point it is useful to reparametrize eq. (10) as

$$f_s L^d \simeq h(L/\xi), \quad (14)$$

with $h(L/\xi) = (L/\xi)^d g(\xi/L)$. Inserting the scaling law $\xi \sim t^{-\nu}$ we obtain

$$f_s \simeq L^{-d} \tilde{h}(L^{1/\nu} t), \quad (15)$$

and, by differentiation with respect to β ,

$$E_s \sim L^{-d+1/\nu} \tilde{h}'(L^{1/\nu} t) \quad (16)$$

and

$$C_s \sim L^{-d+2/\nu} \tilde{h}''(L^{1/\nu} t). \quad (17)$$

For the critical temperature $t = 0$ this means

$$E_s \sim L^{-d+1/\nu}, \quad (18)$$

and

$$C_s \sim L^{-d+2/\nu}. \quad (19)$$

In our numerical study we approximated the nonsingular part of the free energy density by its Taylor expansion, truncated at second order,

$$f_{\text{ns}} \simeq F_{\text{ns}} - E_{\text{ns}} (\beta - \beta_c) - \frac{1}{2} C_{\text{ns}} (\beta - \beta_c)^2, \quad (20)$$

where F_{ns} , E_{ns} and C_{ns} are the nonsingular parts of the free energy density, the energy density and the specific heat at the critical point, respectively.

2 MC Simulations

2.1 Simulations at β_c

We simulated the model at $\beta_c = 0.2216544$ on lattices of size $L = 12$ up to $L = 112$. For the simulation we employed the single cluster algorithm. The updating between two measurements consisted of a number of clusters, ranging between 5 and 50, and a single Metropolis sweep. The total number of measurements was several millions for the smaller lattice and some hundred thousands for the larger systems.

We measured the energy E , the specific heat C and the derivative of C with respect to the inverse temperature β . Our results for E and C are summarised in table 1.

We fitted our data for the energy and the specific heat according to the ansätze

$$E = E_{\text{ns}} + \text{const}_E L^{-d+1/\nu} \quad (21)$$

and

$$C = C_{\text{ns}} + \text{const}_C L^{-d+2/\nu} \quad (22)$$

that are motivated by eqs. (18) and (19), respectively. The results are summarised in table 2. The χ^2 per degree of freedom becomes smaller than one if only lattices with $L \geq 20$ are included in the fit.

One observes that the result for ν obtained from the energy is smaller than that from fitting the specific heat. However, when discarding data from small L the estimate of ν from the energy increases, while that from the specific heat decreases.

Next we fitted the data for the energy and the specific heat simultaneously. We checked that the cross-correlation of the two quantities is small compared to the geometric mean of the variances of the two quantities. Therefore it is justified to treat for simplicity the data as independent. When all data are included into the fit the χ^2 per degree of freedom becomes unacceptably large. Discarding again the $L = 12$ and $L = 16$ data, the fits become very good. It is interesting to note that the value for ν changes only little when $L = 12$ and 16 are discarded from the fit.

In order to check the dependence of our result on the value of the critical coupling, we repeated the fit for $\beta = 0.2216538$ and $\beta = 0.221655$. The values for the energy and the specific

L	E	C
12	0.352212(10)	11.0572(24)
16	0.344859(16)	12.2103(58)
20	0.340931(7)	13.1588(47)
24	0.338489(12)	13.9138(95)
28	0.336873(6)	14.5920(55)
32	0.335721(6)	15.1921(74)
36	0.334882(6)	15.7199(84)
40	0.334233(7)	16.222(19)
44	0.333735(6)	16.652(11)
48	0.333302(10)	17.075(25)
56	0.332701(8)	17.800(21)
64	0.332286(9)	18.483(30)
72	0.331954(9)	19.059(41)
80	0.331720(7)	19.617(32)
96	0.331365(8)	20.517(65)
112	0.331145(8)	21.439(80)

Table 1: Results for the energy E and the the specific heat C at $\beta_c = 0.2216544$ for various lattice sizes L .

data	L_{min}	X	ν	const $_E$	E_{ns}	const $_C$	C_{ns}
energy	12	1.04	0.6280(5)	0.7276(25)	0.330190(7)		
data	16	1.13	0.6282(10)	0.729(5)	0.330192(9)		
only	20	0.86	0.6296(12)	0.737(7)	0.330200(9)		
specific	12	1.42	0.6380(7)			20.9(8)	-18.2(9)
heat data	16	1.35	0.6365(13)			19.3(1.2)	-16.4(1.4)
only	20	0.45	0.6329(16)			16.1(1.3)	-12.9(1.4)
both	12	5.6	0.6316(4)	0.7440(20)	0.330229(5)	15.32(30)	-12.13(33)
data	16	2.25	0.6315(8)	0.7460(40)	0.330218(7)	15.15(54)	-11.83(61)
combined	20	0.75	0.6308(10)	0.7431(52)	0.330209(8)	14.58(66)	-11.12(76)

Table 2: Results of fits of the energy E and the the specific heat C at $\beta_c = 0.2216544$. The upper part gives results from energy data only, the following three rows state results from specific heat data only, while the lower part refers to fits where both sets of data were combined. Only data of simulations with lattice size greater or equal to L_{min} were used for the fits. X denotes χ^2 per degree of freedom.

heat at these β -values were obtained from first order Taylor expansion and the numerically determined values of the derivatives. Taking into account the error induced by the uncertainty of β_c we arrive at the final estimates $E_{\text{ns}} = 0.330209(14)$, $C_{\text{ns}} = -11.1(8)$ and $\nu = 0.6308(10)$ obtained from the combined energy and specific heat fit with $L \geq 20$. Here only statistical errors are given. It is difficult to quantify systematic errors due to corrections to scaling. We tried to use an ansatz that includes a leading correction to scaling term

$$E_s \sim L^{-d+1/\nu} (1 + c L^{-\omega}) , \quad (23)$$

with the correction to scaling exponent $\omega = 0.81(5)$ [3, 6]. It turned out that the amplitude of the correction to scaling term was consistent with zero within errorbars. The estimate of ν was $\nu = 0.631(4)$ when all data for the energy and the specific heat were included in the fit.

Since the estimate of ν obtained from the the fit without corrections to scaling is in nice agreement with recent results given in the literature (for an overview see [7]), we also regard the estimates for E_{ns} and C_{ns} , which will be used in the following, as reliable.

2.2 Simulations at $\beta \neq \beta_c$

Next we simulated the model at temperatures below and above the critical temperature, such that results for the thermodynamic limit could be obtained. The resulting Monte Carlo estimates for E are fitted to

$$E \simeq E_{\text{ns}} - C_{\text{ns}} \beta_c t \mp A_{\pm} \beta_c \frac{|t|^{1-\alpha}}{1-\alpha} , \quad (24)$$

which is obtained by integration of eq. (6). For the simulations in the symmetric phase and for part of the simulations in the broken phase we used the single cluster algorithm [8] combined with a standard local Metropolis update. A typical mixture was 20 cluster updates plus a single Metropolis sweep, followed by a measurement of observables. The total number of measurements was typically of order a few hundred thousands up to two millions. Part of the results for the broken phase were obtained in the course of an other project [9], using a demon program coded in multispin fashion. For details of these simulations we refer to [9].

Our results for E are displayed in table 3. The β -values were chosen in the range 0.218909 to 0.224. The corresponding reduced temperature covers the interval from 0.0124 to -0.011. The typical lattice sizes were 96 and 128. We convinced ourselves that we always reached the thermodynamic limit within the numerical precision. In the table we marked those values that were discarded because of finite size effects by an “F”. Data that were excluded because of a too large distance from criticality are marked with a “T” (see below).

We then made two types of fits: We first fixed β_c and α , and fitted E_{ns} , C_{ns} , A_+ , and A_- . Then we only fixed β_c and fitted all the other parameters in eq. (24). In both cases, we used in addition to the reduced temperature t an alternative definition,

$$t' = \frac{\beta_c}{\beta} - 1 . \quad (25)$$

Comparing the fit results from the two definitions should give us an estimate of systematic effects that stem e.g. from the inclusion of data that have too large t or the neglect of subleading terms in eq. (24). The results for the fit parameters are summarised in table 4.

β	E	L
0.2189088	0.311775(5)	96 T
0.21931	0.313849(14)	80 T
0.2197088	0.315949(6)	96
0.2202	0.318742(11)	100
0.2204	0.319958(6)	96
0.2205	0.320587(9)	128
0.2205	0.320592(9)	96
0.2206	0.321230(11)	128
0.2206	0.321220(8)	96
0.2207	0.321887(9)	128
0.2207	0.321900(8)	96
0.2208	0.322581(9)	128
0.2208	0.322593(9)	96
0.2209	0.323280(5)	128
0.2209	0.323301(8)	96 F
0.2210	0.323995(10)	128
0.2210	0.324040(9)	96 F
0.2220	0.340001(12)	128
0.2220	0.340001(34)	96
0.2221	0.342368(19)	96
0.2222	0.344592(35)	96
0.2224	0.348911(35)	96
0.2226	0.353134(36)	96
0.2228	0.357057(36)	96
0.2229	0.358935(47)	64
0.2230	0.360972(31)	96
0.2234	0.368280(28)	96 T
0.2236	0.371725(27)	96 T
0.2238	0.375248(27)	96 T
0.2240	0.378615(26)	96 T

Table 3: Monte Carlo results for the energy of the 3D off critical Ising model. A “T” in the last column means that the corresponding data is not used for the fits because of its too large reduced temperature. Exclusion of the fits because of finite size effects is indicated by an “F”.

α	type	A_+	A_-	A_+/A_-	E_{ns}	C_{ns}
0.100 f	t	11.194(56)	19.068(42)	0.5871(16)	0.33037(1)	-12.561(96)
	t'	11.147(51)	19.132(41)	0.5826(15)	0.33033(1)	-12.544(88)
0.104 f	t	10.374(52)	18.076(39)	0.5739(17)	0.33034(1)	-11.549(91)
	t'	10.329(47)	18.140(38)	0.5694(15)	0.22030(1)	-11.545(85)
0.108 f	t	9.625(49)	17.160(37)	0.5609(17)	0.33031(1)	-10.613(89)
	t'	9.582(45)	17.224(36)	0.5563(15)	0.33027(1)	-10.601(88)
0.112 f	t	8.940(47)	16.311(34)	0.5481(18)	0.33028(1)	-9.743(85)
	t'	8.900(42)	16.375(33)	0.5435(15)	0.33024(1)	-9.733(78)
0.1115(37)	t	9.03(63)	16.42(77)	0.550(12)	0.33029(3)	-9.86(80)
0.1047(48)	t'	10.19(96)	17.97(1.17)	0.567(16)	0.33030(4)	-11.37(1.17)

Table 4: Results for the fit parameters of eq. (24). An “f” in the first column means that the corresponding parameter was kept fixed to the quoted value. t and t' indicate the definition of reduced temperature that was employed in the fit.

We first started taking all the data of table 3. However, it turned out that in order to have fits with a reasonable level of confidence, we had to discard the data marked with a “T”. The fits with the remaining data (the results of which are quoted in table 4) had a χ^2 per degree of freedom of 0.9 to 1.2.

There is a systematic difference of the fits with the two different definitions of the reduced temperature. In case of the fits with fixed α we could further reduce the data to include only results closer to criticality. This moved a little bit the estimates, however, did not diminish the systematic difference between the t and t' fits. We therefore conclude that in order to cure that problem most likely correction terms should be added in the ansatz eq. (24). To this end, one would probably need more or more precise data.

The slight mismatch of the result for E_{ns} obtained in this section with the result obtained from finite size scaling at the critical point should be attributed to such corrections to scaling and not to a failure of the theoretical prediction.

Using the results for E_{ns} , C_{ns} and ν obtained at the critical point one can compute the scaling amplitude from a single energy value, just by solving eq. (24) with respect to A_+ or A_- . The results are given in table 5.

The main sources of error in the amplitudes A_+ and A_- computed this way are induced by the errors of C_{ns} and ν . However, when taking the ratio A_+/A_- from amplitudes computed at about the same distance from β_c the dependence on ν completely cancels, and also the error by C_{ns} partially cancels. When taking the amplitudes obtained from the β -values closest to β_c we obtain $A_+/A_- = 0.560(10)$, which is nicely consistent with the result that was obtained using only data with $\beta \neq \beta_c$.

Let us now make a comparison with a few results of the literature. Estimates from ϵ -expansion, field theoretic calculations in $D = 3$, high temperature expansions and from experiments are given in [10]. For the readers convenience, we reproduce part of that table in our table 6 and complete it with our present estimates. Apparently, our estimates are larger than the other ones cited in the table. However our most accurate estimate MC, (c) is consis-

β	A_+
0.2204	9.86(41)(18)
0.2205	9.85(40)(19)
0.2206	9.85(40)(19)
0.2207	9.84(39)(19)
0.2208	9.82(39)(20)
0.2209	9.82(39)(20)
0.2210	9.82(38)(20)
β	A_-
0.2220	17.55(36)(46)
0.2221	17.56(37)(39)
0.2222	17.52(37)(37)
0.2224	17.50(39)(36)
0.2226	17.53(40)(35)
0.2228	17.49(41)(34)

Table 5: Estimates for the amplitudes A_{\pm} based on the estimates $E_{\text{ns}} = 0.330209(14)$, $C_{\text{ns}} = 11.1(8)$ and $\nu = 0.6308(10)$. The estimates are obtained by solving eq. (24) with respect to A_+ or A_- a fixed β , assuming hyperscaling $\alpha = 2 - d\nu$. The dominant sources of error in the resulting amplitudes are the errors of C_{ns} and ν . These errors are displayed in the first and second brackets respectively.

method	A_+/A_-	reference	year
ϵ -expansion	0.524(10)	[11]	85/86
ϵ -expansion	0.547(21)	[10]	96
field theory $D = 3$	0.541(14)	[12]	87
field theory $D = 3$	0.536(19)	[10]	96
HT,LT series	0.523(9)	[1]	89
MC, (a)	0.550(12)	this work	97
MC, (b)	0.567(16)	this work	97
MC, (c)	0.560(10)	this work	97

Table 6: Amplitude ratio estimates taken from the literature and from this work. The estimate (a) and (b) are the fit results quoted in table 4, and discussed in section 2.2. Estimate (a) was obtained by including also information from the data at the critical point, cf. the discussion at the end of section 2.2. Some estimates from experiments are 0.56(2) (binary mixtures), 0.49-0.53 (liquid-vapour systems), and 0.49-0.54 (magnetic systems), see ref. [2].

tent within error-bars with the most recent result from ϵ -expansion [10] and the results from renormalized perturbation theory in three dimensions [12, 10]. We think that the disagreement with the estimate based on high and low temperature expansion is most likely due to an under-estimation of the error in ref. [1].

3 The universal constant $f_s \xi^d$

In this section we try to extract the numerical value of $f_s \xi^d$ in both phases of the model. The values for the second moment correlation length ξ_{2nd} are taken from ref. [13].

The estimates for f_s at given β -values were obtained in the following way: We took $E - E_{ns} - C_{ns}(\beta - \beta_c)$ as an approximation of the singular part of the energy. The constants E_{ns} and C_{ns} were taken from the combined energy and specific heat fit at the critical point. Then we computed f_s as the integral over β of the singular part of the energy. We interpolated the singular part of energy for β -values not simulated with the scaling ansatz, where we use $\nu = 0.6308$ and the amplitude was computed from the closest β -value simulated. The results are given in table 7.

In both phases we just have results for two β -values. Since the results of these two β -values nicely agree we regard the results $f_s \xi^3 = 0.0355(15)$ and $f_s \xi^3 = 0.0085(2)$ for the high and low temperature phase as reliable estimates for the critical limits.

Note that the result depends on the normalisation chosen here, in particular we have chosen to take the free energy per link rather than per site.

4 Conclusion

By a careful scaling and finite size scaling analysis of energy and specific heat data we obtained estimates for various critical quantities. Taking into account the simplicity of the approach,

β	$\xi_{2\text{nd}}$	f_s	$f_s \xi_{2\text{nd}}^3$
0.21931	8.760(5)	0.0000524(22)	0.0352(15)
0.22020	11.877(7)	0.0000212(9)	0.0355(15)
0.22311	6.093(9)	0.0000377(9)	0.0085(2)
0.2240	4.509(6)	0.0000927(22)	0.0085(2)

Table 7: In the second column we give results of ref. [13] for the second moment correlation length $\xi_{2\text{nd}}$. In the third column we give our estimate for the singular part of free energy density f_s , while the fourth column gives the resulting estimate for the universal combination $f_s \xi_{2\text{nd}}^3$.

especially the results for the exponents ν and α are remarkably precise.

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